

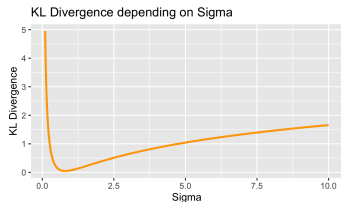
Introduction to Machine Learning

Kullback-Leibler Divergence



Learning goals

- Know the KL divergence as distance between distributions
- Understand KL as expected log-difference
- Understand how KL can be used as loss
- Understand that KL is equivalent to the expected likelihood ratio



KULLBACK-LEIBLER DIVERGENCE

We now want to establish a measure of distance between (discrete or continuous) distributions with the same support for $X \sim p(X)$:

$$D_{KL}(p||q) = \mathbb{E}_{X \sim p} \left[\log \frac{p(X)}{q(X)} \right] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)},$$

or:

$$D_{KL}(p||q) = \mathbb{E}_{X \sim p} \left[\log \frac{p(X)}{q(X)} \right] = \int_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} dx.$$

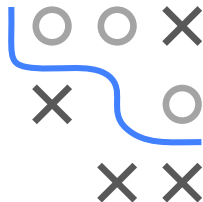
In the above definition, we use the conventions that $0 \log(0/0) = 0$, $0 \log(0/q) = 0$ and $p \log(p/0) = \infty$ (based on continuity arguments where $p \rightarrow 0$). Thus, if there is any realization $x \in \mathcal{X}$ such that $p(x) > 0$ and $q(x) = 0$, then $D_{KL}(p||q) = \infty$.



KULLBACK-LEIBLER DIVERGENCE / 2

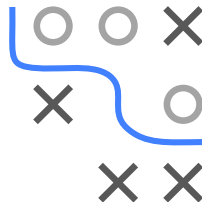
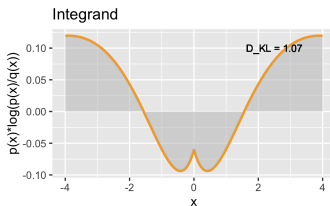
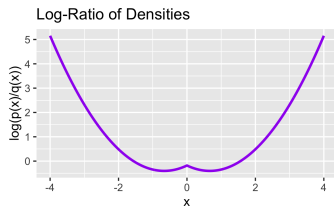
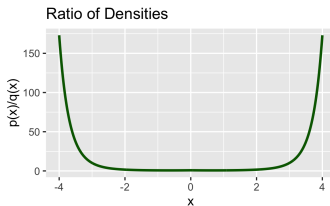
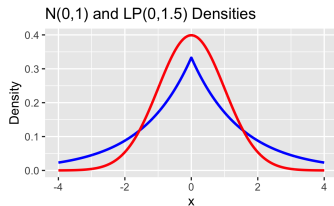
$$D_{KL}(p||q) = \mathbb{E}_{X \sim p} \left[\log \frac{p(X)}{q(X)} \right]$$

- What is the intuition behind this formula?
- We will soon see that KL has quite some value in measuring “differences” but is not a true distance.
- We already see that the formula is not symmetric and it often makes sense to think of p as the first or original form of the data, and q as something that we want to measure the quality of with reference to p .



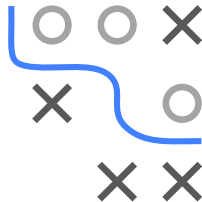
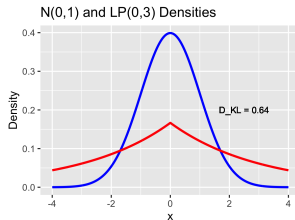
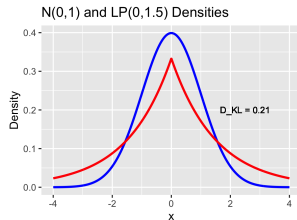
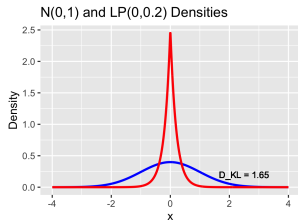
KL-DIVERGENCE EXAMPLE

KL divergence between $p(x) = LP(0, 1.5)$ and $q(x) = N(0, 1)$ is different since KL not symmetric



KL-DIVERGENCE EXAMPLE

KL divergence of $p(x) = N(0, 1)$ and $q(x) = LP(0, \sigma)$ for varying σ



INFORMATION INEQUALITY

$D_{KL}(p||q) \geq 0$ holds always true for any pair of distributions, and holds with equality if and only if $p = q$.

We use Jensen's inequality. Let A be the support of p :

$$\begin{aligned} -D_{KL}(p||q) &= -\sum_{x \in A} p(x) \log \frac{p(x)}{q(x)} \\ &= \sum_{x \in A} p(x) \log \frac{q(x)}{p(x)} \\ &\leq \log \sum_{x \in A} p(x) \frac{q(x)}{p(x)} \\ &\leq \log \sum_{x \in \mathcal{X}} q(x) = \log(1) = 0 \end{aligned}$$

As \log is strictly concave, Jensen also tells us that equality can only happen if $q(x)/p(x)$ is constant everywhere. That implies $p = q$.



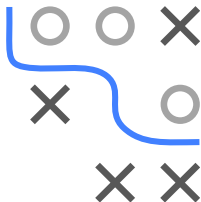
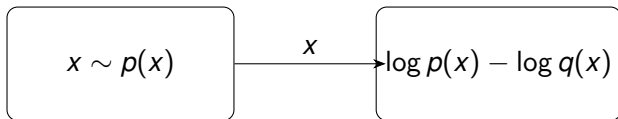
KL AS LOG-DIFFERENCE

Suppose that data is being generated from an unknown distribution $p(x)$ and we model $p(x)$ using an approximating distribution $q(x)$.

First, we could simply see KL as the expected log-difference between $p(x)$ and $q(x)$:

$$D_{KL}(p||q) = \mathbb{E}_{x \sim p}[\log(p(x)) - \log(q(x))].$$

This is why we integrate out with respect to the data distribution p . A “good” approximation $q(x)$ should minimize the difference to $p(x)$.



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A 3x3 grid with a blue path starting at the top-left cell (0,0) and ending at the bottom-right cell (2,2). The path is composed of three segments: a vertical segment from (0,0) to (0,1), a horizontal segment from (0,1) to (1,1), and a diagonal segment from (1,1) to (2,2). The cells (0,1), (1,0), (1,1), and (2,0) are marked with a grey 'X', while the cells (0,2), (1,2), and (2,1) are marked with a grey circle.

The figure consists of four subplots arranged in a 2x2 grid, illustrating the relationship between a standard normal distribution $N(0, 1)$ and a Laplace distribution $LP(0, 3)$.

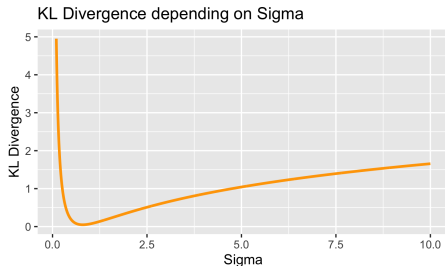
- Top Left:** Titled "N(0, 1) and LP(0,3) Densities". It shows the probability density functions of both distributions. The blue curve represents the $N(0, 1)$ density, which is centered at 0 with a peak density of approximately 0.4. The red curve represents the $LP(0, 3)$ density, which is also centered at 0 but has a much flatter peak density of approximately 0.17. The x-axis ranges from -4 to 4, and the y-axis (Density) ranges from 0.0 to 0.4.
- Top Right:** Titled " $\log(p(x)) - \log(q(x))$ ". It shows the log-density difference between the two distributions. The blue curve represents the $N(0, 1)$ log-density, and the red curve represents the $LP(0, 3)$ log-density. The shaded gray area represents the difference between them. The x-axis ranges from -4 to 4, and the y-axis (Log-Density) ranges from -7.5 to -2.5.
- Bottom Left:** Titled " $E[\log(p(x))] - E[\log(q(x))]$ ". It shows the expectation difference between the two distributions. The blue curve represents the $N(0, 1)$ expectation, and the red curve represents the $LP(0, 3)$ expectation. The shaded gray area represents the difference between them. The x-axis ranges from -4 to 4, and the y-axis (Expectation Difference) ranges from -0.6 to 0.0. A text label indicates $D_{KL} = 0.64$.
- Bottom Right:** Titled " $E[\log(p(x)/q(x))]$ ". It shows the expectation ratio between the two distributions. The orange curve represents the expectation ratio. The shaded gray area represents the difference between the two distributions. The x-axis ranges from -4 to 4, and the y-axis (Expectation Ratio) ranges from 0.0 to 0.3. A text label indicates $D_{KL} = 0.64$.

KL IN FITTING

In machine learning, KL divergence is commonly used to quantify how different one distribution is from another.

Because KL quantifies the difference between distributions, it can be used as a loss function between distributions.

In our example, we investigated the KL between $p = N(0, 1)$ and $q = LP(0, \sigma)$. Now, we identify an optimal σ which minimizes the KL.



KL AS LIKELIHOOD RATIO

- Let us assume we have some data and want to figure out whether $p(x)$ or $q(x)$ matches it better.
- How do we usually do that in stats? Likelihood ratio!

$$LR = \prod_i \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})} \quad LLR = \sum_i \log \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})}$$

If for $\mathbf{x}^{(i)}$ we have $p(\mathbf{x}^{(i)})/q(\mathbf{x}^{(i)}) > 1$, then p seems better, for $p(\mathbf{x}^{(i)})/q(\mathbf{x}^{(i)}) < 1$ q seems better.

- Now assume that the data is generated by p . Can also ask:
- "How to quantify how much better does p fit than q , on average?"

$$\mathbb{E}_p \left[\log \frac{p(X)}{q(X)} \right]$$

That expected LLR is really KL!

